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Numerical simulations of electron field emitters based on hemi-ellipsoid geometry

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ABSTRACT

In order to evaluate the electric field associated to field emission, a computational model was elaborated to investigate hemi-ellipsoidal structures. The emitters were simulated both as 2D single structures and forming arrays, aiming to establish a relevant methodology for a more complex research.

1. Introduction

Previous researches performed in the past decades revealed that vacuum electronic devices are again competitive with solid-state semiconductor devices, but this time using the field emission phenomena [1]. Among the advantages are the low cost manufacturing and the ability to operate with high current density [2]. The field emission devices have been thoroughly studied, as well as differences in the shape and materials used. Latest researches have demonstrated that carbon nanotubes (CNTs) present excellent quality as electron emitters: mechanical robustness, high electrical conductivity and low cost manufacturing. As the manufacturing processes are very well controlled, CNT arrays are precisely built with the desired geometric parameters, such as height, radius and density of emitters.

2. Theory

The theory related to field emission was firstly studied in 1928 by Fowler and Nordheim [3–5]. The emitted current density J_{FN} (A/cm^2) is related to the electric field on the surface E (V/cm) and to the work function, ϕ (eV), according to equation (1), which is also known as the Fowler-Nordheim Relationship (F–N).

$$J_{FN} = \frac{AE^2}{\phi t^2(y)} \exp\left(-B\frac{\phi^{3/2}}{E} v(y)\right) \quad (1)$$

where:

$$A = 1.54 \times 10^{-6} \text{A eV} / \text{V}^2;\ \ B = 6.87 \times 10^{7} (\text{V eV})^{-3/2} / \text{cm};$$

$$y = 3.79 \times 10^{-4} E^{1/2} / \phi$$

$$t^2(y) = 1.1;\ v(y) = 0.95 - y^2$$

The emitted current - I (A) - can be calculated by integrating the current density - J_{FN} - over the surface of the emitter–S –, just as shown in (2).

$$I = \iint_{\text{emitter}} J_{FN} dS \quad (2)$$

The macroscopic electric field F_M is defined by the ratio between anode-cathode voltage, V_{anode}, and the anode-cathode distance, d. Due to the protruding shape of the emitter, the electric field E on its surface is significantly higher than the applied macroscopic field

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F_M. The ratio between E and F_M is known as the field enhancement factor, γ [2].

Various studies have demonstrated that some geometries present higher γ than others, producing higher current densities with smaller V_{anode}, which is a characteristic of a good emitter. It is considered as an ideal emitter geometry the classical model of a sphere floating over a cathode (both at the same potential) [6] – even though a floating sphere obviously cannot be manufactured. A geometry that presents good γ and works with satisfactory mechanical stability is the hemi-ellipsoid. This structure can be modeled rotating an ellipse arc on its major semi-axis. Equation (3) provides the field enhancement factor, γ, at the apex of a hemi-ellipsoidal emitter of height L and base radius ρ [7].

$$\gamma = \frac{\zeta^3}{[\{\alpha \ln(\alpha + \zeta)\} - \zeta]} \tag{3}$$

where: $\zeta = (\alpha^2 - 1)^{1/2}$, $\alpha = L/\rho$

Arrays of hemi-ellipsoidal emitters were also simulated. In these cases the screening effect occurs [8], which provokes distortion of the field surrounding the emitters and it also changes the magnitude of γ.

3. Methodology

The numerical simulations were performed using the Ansys-Maxwell software [9], which applies the finite elements method to solve and determine electric field distribution. During the simulations the electrodes were configured as perfect electrical conductors (PEC) and considered immersed into perfect vacuum.

Some structures were introduced nearby the emitters to improve the mesh refinement in the critical regions of the model. Although these structures were configured as vacuum and did not influence the electric field, they induce the software to increment the mesh density within the critical regions.

A virtual cathode was designed surrounding the apex of the hemi-ellipsoidal emitters to the computation of I. This new element consists of a surface with negligible thickness, equidistant and near the emitter real surface. The numerical simulations could not calculate the current - as shown in (2) - because the real cathode was at zero potential, impeding the integration of the current density over the surface. Thereby, I was computed by integrating J_{FN} over the virtual cathode.

Emitters with base radius greater than 150 nm were considered not very effective, since they presented very low aspect ratios (L/ρ) and, consequently, low values of γ. Base radius smaller than 40 nm were avoided because emitters with high aspect ratios can be studied as if they were CNTs of great height—what would simplify the analysis—once the mesh generation for hemi-ellipsoidal geometries is always more complex. Therefore, this study evaluated the base radius values within the interval of interest defined between 40 nm and 150 nm. The height was kept constant at 1000 nm. Complementally, the work function was set at 5 eV and the anode voltage was used as $V_{anode} = 1000$ V in all simulations.

4. Obtained results

4.1. 2D single hemi-ellipsoidal emitter

The simulated structure is shown in Fig. 1(a) and it is important to emphasize that only half of the structure design is necessary because the software automatically considers a revolution over the Z symmetry axis. In Fig. 1(b), the half apex of the hemi-ellipsoidal emitter along with the virtual probe for calculating E positioned at its tip is presented. There is an ellipse surrounding the emitter surface (at a distance of 2 nm) which delimits the region aimed for the applied mesh operation. Inside this region the additional operation makes the software generate smaller elements, increasing the mesh density and minimizing numerical noise. The dimensions for the entire model are listed in Table 1.

The field enhancement factor at the emitter apex—γ — is presented in Fig. 2 as a function of ρ. The solid line represents the simulation results, while the dashed line depicts equations (3)–(5) for hemi-ellipsoidal emitter—which were obtained from literature [7,10,11]. It is important to mention that these three equations result into coinciding lines (shown in Fig. 2); however, other not less important consideration is that the solid line presents a similar behavior.

$$\gamma = \frac{\left(\lambda^2 - 1\right)^{1.5}}{\lambda \ln\left[\lambda + \left(\lambda^2 - 1\right)^{1/2}\right] - \left(\lambda^2 - 1\right)^{1/2}} \tag{4}$$

where: $\lambda = L/\rho$

$$\gamma = \frac{2\xi^3}{\left(1 - \xi^2\right)\left(\ln\frac{1+\xi}{1-\xi} - 2\xi\right)} \tag{5}$$

where. $\xi = \sqrt{1 - \frac{\rho^2}{L^2}}$

Considering a voltage $V_{anode} = 1000$ V and a distance d = 10 μm, the resulting macroscopic field is $F_M = 1 \times 10^8$ V/m. Now, taking into account $\rho = 100$ nm, the electric field established at the apex is 4.10×10^9 V/m (simulated), thereby, $\gamma = 41$. This hand-calculated result is equal to the simulated one found in Fig. 2 (marker "m6") and it is in accordance with the literature, where $\gamma = 49$ (marker "m5").

In Fig. 3, γ is presented as a function of d, for a specific emitter with $\rho = 100$ nm. It is possible to observe that γ is approximately constant for $d \geq 10$ μm.

The distribution of γ as a function of the emitting surface angle θ ($\theta = 0°$ corresponds to the apex) is represented in Fig. 4. The radius was again set to $\rho = 100$ nm. It can be noted the marker "m1" highlighting the value of γ specifically at the apex on the graph; moreover, this value is in accordance with the simulated result from Fig. 2.

Computational simulations were performed to investigate the behavior of emitters with aspect ratio (L/ρ) in the range of 1–80. Regarding these models, the parameters d = 100 μm and $\rho = 100$ nm were kept constant, as L was modified between 100 nm and 8000 nm. Fig. 5 presents γ at the apex as a function of the emitter aspect ratio; the simulation result (solid line) can be seen along with the three coinciding curves (3, 4, 5) (dashed line). For a unitary aspect ratio ($L/\rho = 1$), which corresponds to a hemisphere, the exact value $\gamma = 3$ is obtained. If the aspect ratio equals 10 and $\rho = 100$ nm, then $\gamma = 41$ which is again in accordance with the result from Fig. 2.

It is important to evince how close the solid and dashed lines are, even though they start to diverge for larger aspect ratios (see Fig. 5). The percent deviation between simulated and analytical γ is shown in Fig. 6. In other words, considering the parameters $L/\rho = 10$ and $\rho = 100$ nm, the percent deviation between simulated and analytical γ is approximately −16%.

We used a model with the following parameters to investigate the emitted current I: d = 10 μm, L = 1 μm, $\rho = 100$ nm. The virtual cathode described previously was used by the software to calculate I as a function of V_{anode}, whose result can be seen in Fig. 7. Inside the graph, the marker "m1" underlines the point where 1 nA is